Electronic supplementary materials *Mendeleev Commun.*, 2021, **31**, 701–703

The synthesis and copolymerization of 4-hydroxybenzylglycolide: experimental and theoretical aspects

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Contents

S1. Materials and Methods

S1.1. Materials

All the synthetic and polymerization experiments were performed under argon atmosphere. Tetrahydrofuran (THF) and diethyl ether (Et_2O, Merck, Darmstadt, Germany) were refluxed over Na/benzophenone and distilled prior to use. Dichloromethane CH_2Cl_2 (Prime Chemicals Group, Moscow, Russia) was washed with aqueous Na_2CO_3, stirred with $CaCl_2$ powder, refluxed over CaH_2 for 8 h and distilled. (*S*)-Lactide and *rac*-lactide (Merck, Darmstadt, Germany) were purified by recrystallization from toluene and sublimation. Acetonitrile (MeCN), *n*-heptane, ethyl acetate (EtOAc), pyridine, *N*-ethyl-*N*-isopropylpropan-2-amine (DIPEA), 5% Pd/C and Celite 545 were used as purchased (Merck, Darmstadt, Germany). 2,6-Di-*tert*-butyl-4-methylphenoxy magnesium complex $[(BHT)Mg(\mu\text{-}OBn)(THF)]_2$ (BHT-Mg)[23] and 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD)[24] were synthesized according to the literature procedures.

$CDCl_3$ (D 99.8%, Cambridge Isotope Laboratories, Inc., Cambridge, MS, USA) was distilled over P_2O_5 and stored over 4 Å molecular sieves. DMSO-d_6 (D 99.8%, Cambridge Isotope Laboratories, Inc., Cambridge, MS, USA) was used as purchased.

S1.2. Instruments and methods

The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra were recorded on a Bruker AVANCE 400 spectrometer (Bruker, Billerica, MS, USA). The chemical shifts were reported relative to the solvent residual peaks ($CDCl_3$: δ = 7.26 ppm for ^1H NMR spectra and 77.16 ppm for ^{13}C NMR spectra; DMSO-d_6: δ = 2.50 ppm for ^1H NMR spectra and 39.52 ppm for ^{13}C NMR spectra).

Gel permeation chromatography (GPC) measurements of the polymers were performed in THF at a flow rate of 1 ml min^{-1} at 30 °C using an 1260 Infinity II (Agilent Technologies, Santa Clara, CA, USA) integrated instrument equipped with PLgel MIXED-C column (2×10^2 – 2×10^6 Da), autosampler and RI-detector. Calibration was achieved using polystyrene standards.

Elemental analysis (C, H, N, O) was performed on a Perkin Elmer Series II CHNS/O Analyzer 2400 (Perkin Elmer, Waltham, MS, USA).

S2. Synthesis and NMR spectra of 1 and 2

*S2.1. (S)-3-(4-benzyloxybenzyl)-1,4-dioxane-2,5-dione **1***

Compound **1** was synthesized using modified literature procedure.[21] α-Bromoacyl bromide (20.2 g, 0.1 mol) was added to cooled (0 °C) solution of pyridine (8.1 ml, 0.1 mol) and (*S*)-3-(4-benzyloxyphenyl)-2-hydroxypropanoic acid (27.2 g, 0.1 mol) in CH_2Cl_2 (150 ml). The mixture was allowed to warm to room temperature and was stirred for 1 h. Ice water (100 ml) was added, organic phase was separated, washed with 5% HCl (30 ml) and water (2×30 ml). After drying over $MgSO_4$, the organic phase was evaporated under reduced pressure. The product was dissolved in MeCN (250 ml), this solution was added within 1 h at 60 °C with stirring to the solution of DIPEA (17.4 ml, 0.1 mol) in MeCN (500 ml). After 20 min, the solvent was removed, the residue was suspended in EtOAc (200 ml) and filtered, the precipitate was washed by EtOAc (2×50 ml). The combined organic phase was washed with water, 5% HCl, water and dried over $MgSO_4$. The solvent was removed under reduced pressure, and the residue was purified by flash chromatography (silica, CH_2Cl_2). The yield was 24.4 g (78%), colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.41 (m, 5H); 7.18 (2H); 6.96 (2H) {AA'BB', ^3J = 8.6 Hz}; 5.21 (t, ^3J = 4.6 Hz, 1H); 5.06 (s, 2H); 4.56 (d, ^2J = 16.9 Hz, 1H); 3.70 (d, ^2J = 16.9 Hz, 1H); 3.31 (d, ^2J = 4.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 165.09; 163.28; 158.81; 136.67; 131.38; 128.78; 128.25; 127.66; 125.64; 115.78; 70.19; 64.82; 37.81. ^{1}H and ^{13}C NMR spectra of **1** are presented in Figures S1 and S2, respectively.

S2.2. (S)-3-(4-Hydroxybenzyl)-1,4-dioxane-2,5-dione 2

Compound **1** (3.449 g, 11.04 mmol), Pd/C (5 wt %, 0.448 g, 0.421 mmol, 3.7 mol %) and EtOAc (50 ml) were placed into a two-necked round-bottom flask (100 ml). The mixture was heated to 50 °C with stirring, molecular hydrogen (~1 dm^3) was bubbled within 1 h. Then, the mixture was allowed to cool to the room temperature, and stirred under hydrogen atmosphere for 12 h. Most of the product precipitated, preheated EtOAc (4×50 ml) was used to dissolve the crystals. The solution was filtered throw Celite 545 (1 cm) and evaporated under reduced pressure. The yield was 2.346 g (96%), white crystalline powder, m.p. 162 °C. For $C_{11}H_{10}O_5$ calculated (%): C, 59.46; H, 4.54; O, 36.00. Found (%): C, 59.53; H, 4.58; O, 35.89. ^{1}H NMR (DMSO-d_6, 20 °C) δ: 9.36 (s, 1H, –OH); 7.09 (2H); 6.73 (2H) {AA'BB', ^3J = 8.4 Hz}; 5.45 (dd, ^3J = 4.1 & 8.1 Hz, 1H); 5.15 (d, ^2J = 16.1 Hz, 1H); 4.74 (d, ^2J = 16.1 Hz, 1H); 3.22 (dd, ^2J = 14.9 Hz, ^3J = 4.1 Hz, 1H); 3.02 (dd, ^2J = 14.9 Hz, ^3J = 8.1 Hz, 1H). ^{13}C NMR (DMSO-d_6, 20 °C) δ: 166.65; 165.65; 156.45; 130.68; 125.47; 115.22; 115.13; 75.87; 65.68; 35.13. ^{1}H and ^{13}C NMR spectra of **2** are presented in Figures S3 and S4, respectively.

*S2.3. NMR spectra of **1** and **2***

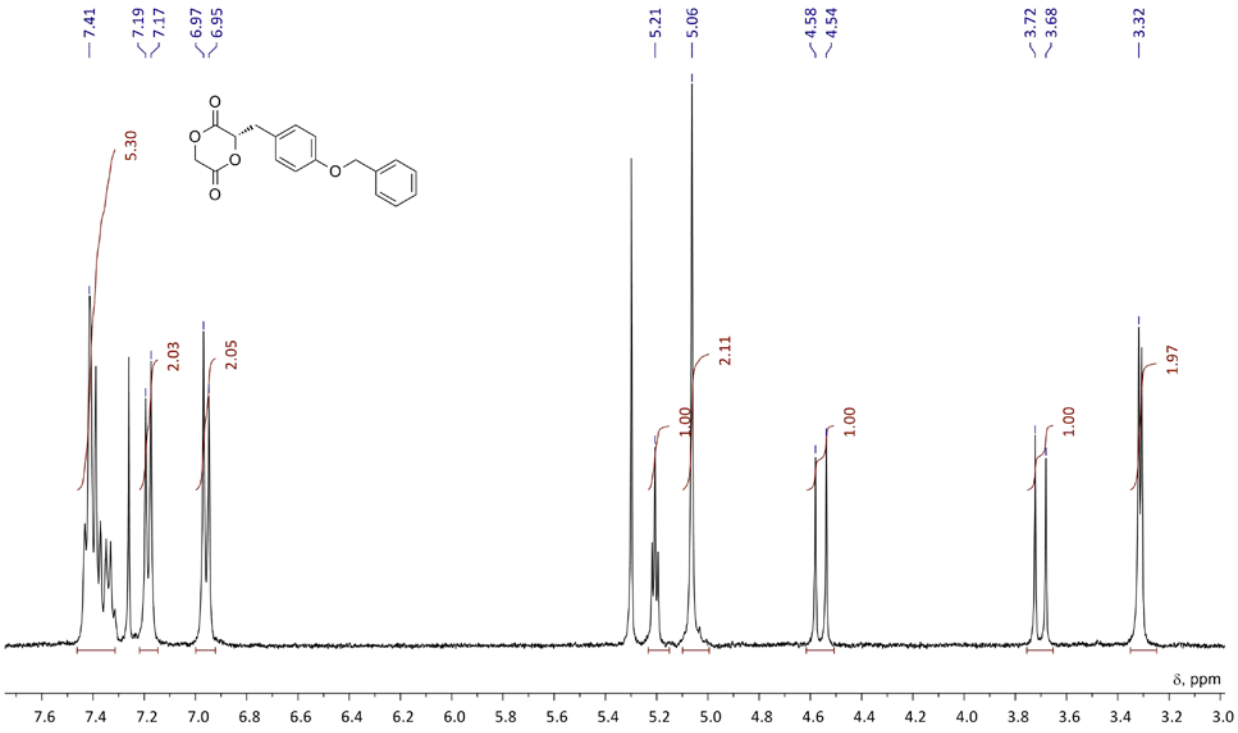


Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 20 °C) of **1**

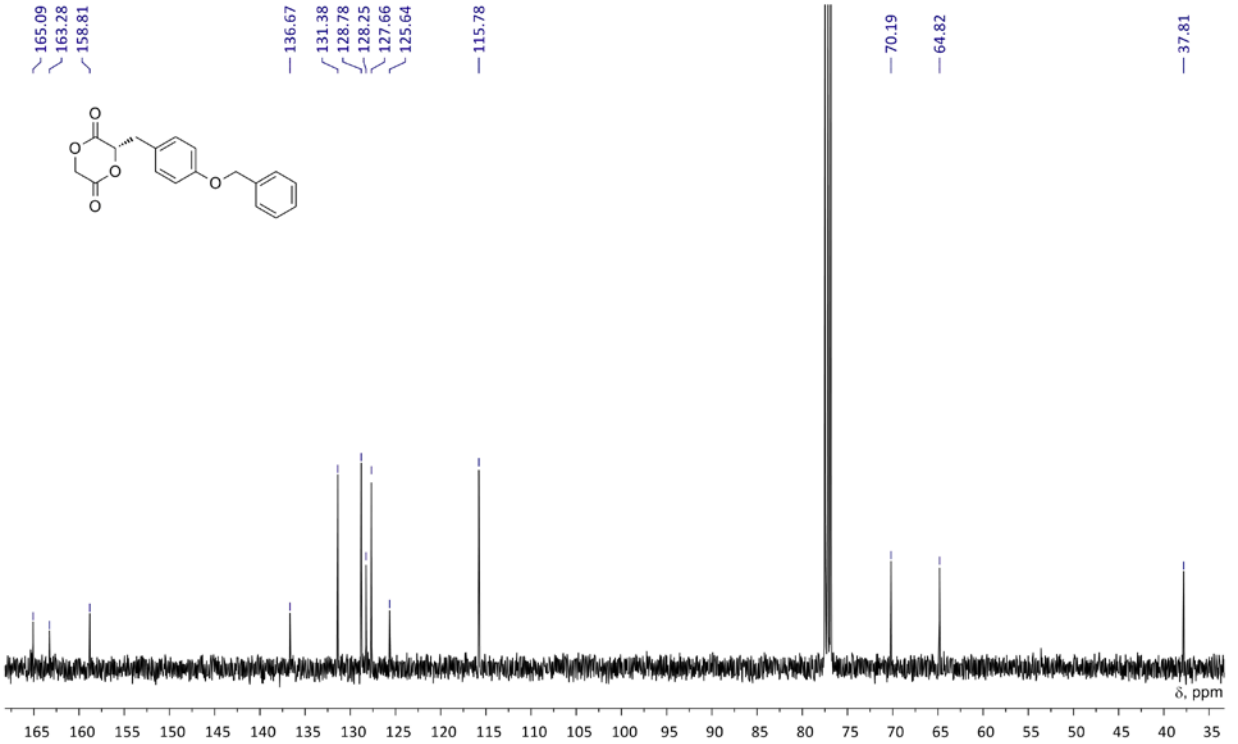


Figure S2. ^{13}C NMR spectrum ($CDCl_3$, 20 °C) of **1**

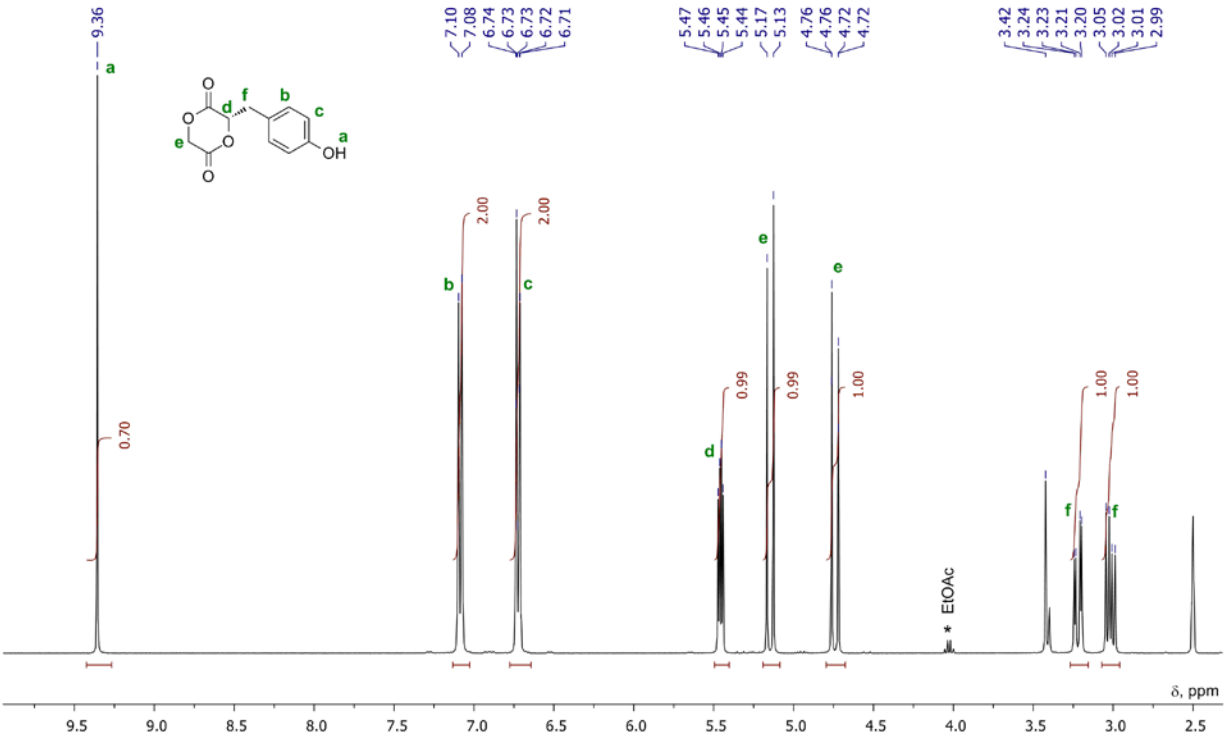


Figure S3. ^{1}H NMR spectrum (DMSO-d_6, 20 °C) of **2**

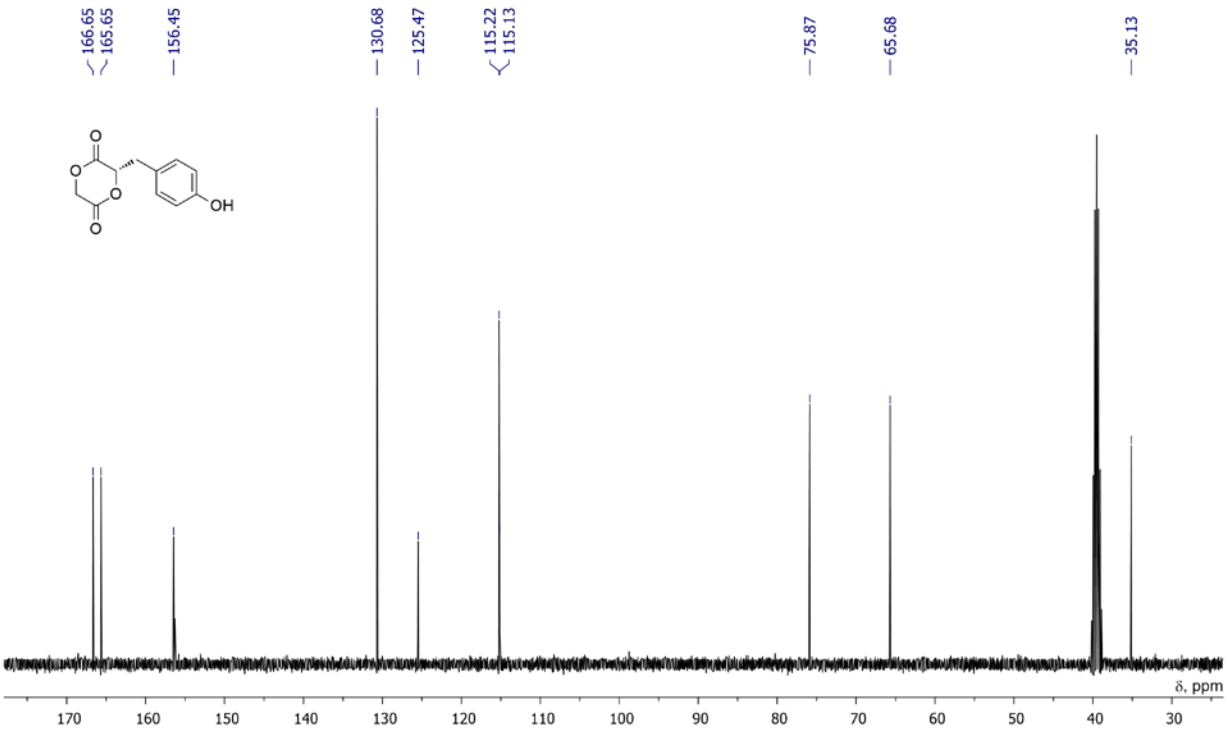


Figure S4. ^{13}C NMR spectrum (DMSO-d_6, 20 °C) of **2**

S3. NMR spectra of copolymers

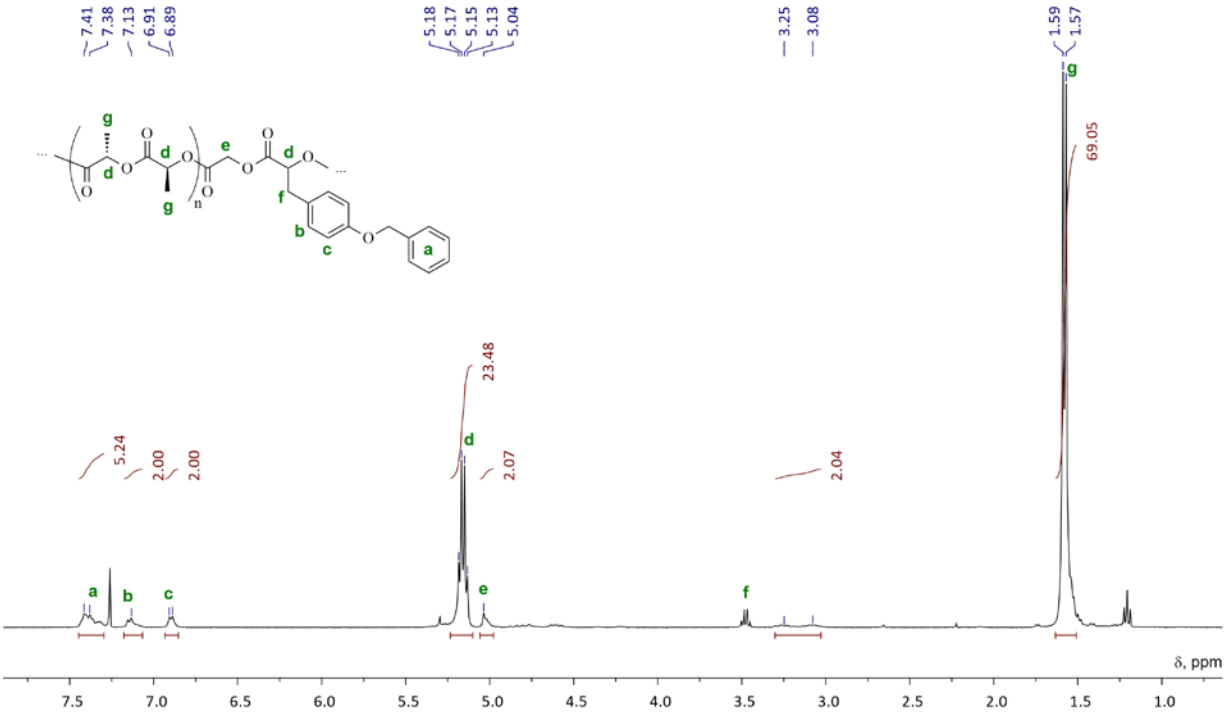


Figure S5. ^{1}H NMR spectrum ($CDCl_3$, 20 °C) of the copolymer of **1** with (*S*)-LA (Table 1, entry 1)

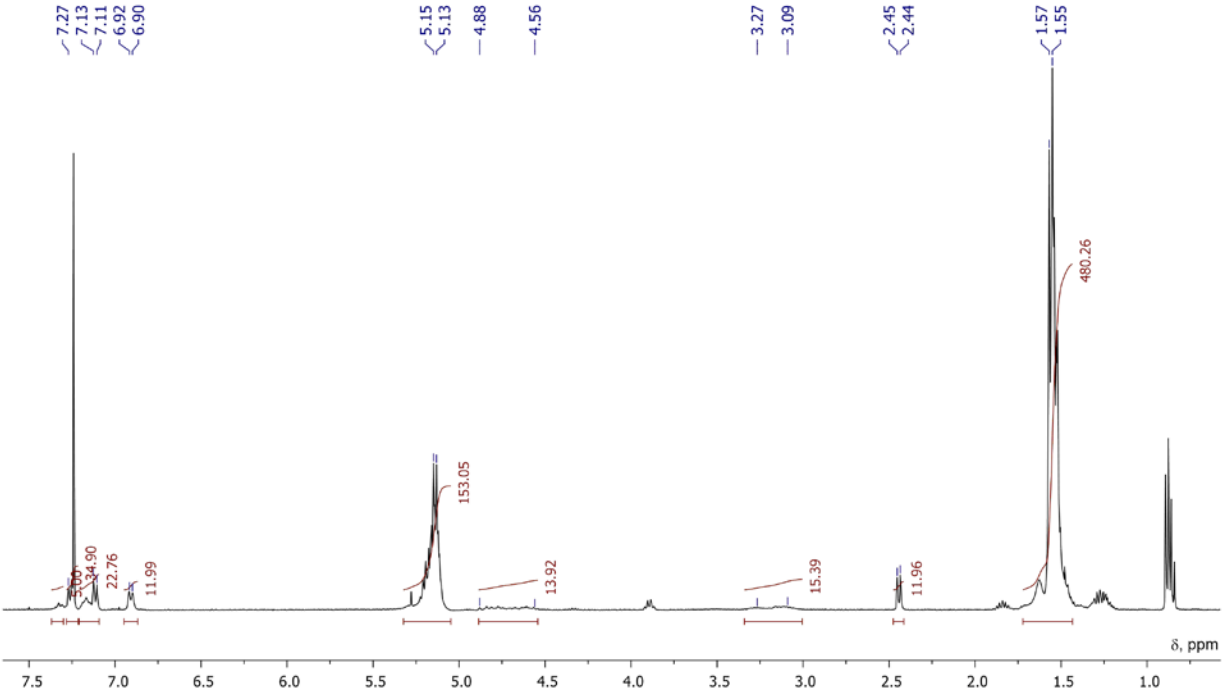
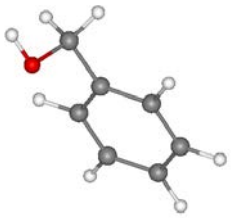


Figure S6. ^{1}H NMR spectrum ($CDCl_3$, 20 °C) of the copolymer of **2** with *rac*-LA (Table 1, entry 7)

S4. DFT calculations data

T = 298.150 K

BnOH



E = -346.466087 E0 = -346.337209

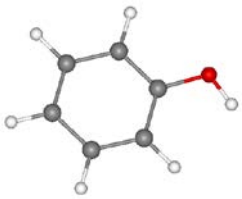
ZPVE = 0.128878 a.u. = 80.8721 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	17.6023	39.9476	0.8887	1.4812	-10.4291
rotational	12.6217	28.0629	0.8887	0.8887	-7.4782
vibrational	2.2059	12.1454	83.1863	83.1863	79.5651
total	32.4299	80.1559	84.9637	85.5562	61.6578

cartesian

8	0.58915430	0.94832873	-0.25546217	6	3.68555403	3.69034743	-1.85082209
6	0.31971157	2.03908825	-1.16278315	1	2.20463324	3.79554987	-0.28134108
1	-0.25115761	0.72761923	0.18159214	6	3.17734790	2.19452643	-3.68253183
1	-0.42243955	1.73442674	-1.92275465	1	1.30083525	1.13317430	-3.53882074
1	-0.08643399	2.90619850	-0.61082339	1	4.35244370	4.41002703	-1.37435305
6	1.60913563	2.42630172	-1.83930826	6	4.03686094	3.11450171	-3.07548165
6	2.47807050	3.34797525	-1.23877978	1	4.97788572	3.38388658	-3.55656958
6	1.97087443	1.85407984	-3.06634521	1	3.44657087	1.74351859	-4.63846111

PhOH



E = -307.206745 E0 = -307.105201

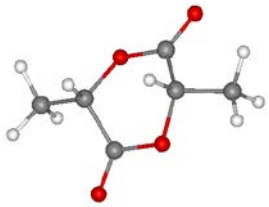
ZPVE = 0.101544 a.u. = 63.7197 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	17.3939	39.5335	0.8887	1.4812	-10.3057
rotational	12.0430	26.9128	0.8887	0.8887	-7.1353
vibrational	1.3720	8.7429	65.5135	65.5135	62.9068
total	30.8089	75.1891	67.2909	67.8834	45.4658

cartesian

6	-1.79676819	1.49498141	2.81906462	1	-0.32640886	2.16650939	5.81214380
6	-0.83460408	1.48678291	3.83703470	6	-2.27724457	2.87718034	5.20966768
6	-2.99808598	2.19428349	2.99688864	1	-4.17032480	3.42307711	4.31981564
6	-3.23254919	2.88144231	4.19042063	1	-2.46247530	3.41423225	6.13948870
1	-3.74879169	2.20048690	2.20245838	8	-1.50938702	0.80039114	1.66725028
6	-1.08029711	2.17676139	5.02399445	1	-2.26198053	0.89577228	1.05766451
1	0.09387047	0.93770075	3.68118000				

***L*-LA**



E = -533.970677 E0 = -533.835400

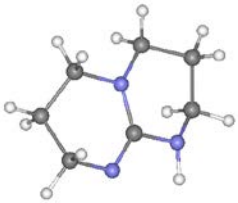
ZPVE = 0.135277 a.u. = 84.8877 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	18.0334	40.8044	0.8887	1.4812	-10.6846
rotational	13.3088	29.4283	0.8887	0.8887	-7.8853
vibrational	5.5010	25.3935	89.1994	89.1994	81.6284
total	36.8433	95.6262	90.9769	91.5694	63.0584

cartesian

8	-1.70498228	-1.43944621	1.42528486	1	0.13619733	0.95675147	1.54007065
6	-0.97402692	-0.71604657	0.78993660	6	0.84472370	-0.81373477	2.55805254
8	-1.27779245	-0.37184727	-0.49440914	8	1.90169930	0.33533621	-1.81141257
6	0.32819700	-0.11031187	1.32005191	1	1.76921964	-0.33399808	2.90139699
6	-0.41867590	0.61788207	-1.14248514	1	1.04285407	-1.87059379	2.34311295
8	1.37564588	-0.17771387	0.30222839	1	0.09139156	-0.75946641	3.35244513
6	1.05618453	0.25479102	-0.95124310	1	-0.21420670	1.44765687	-3.11164856
6	-0.82324243	0.69333720	-2.60017514	1	-1.88217449	0.96729374	-2.67977500
1	-0.59052205	1.59265614	-0.64832479	1	-0.66049409	-0.27254713	-3.09310555

TBD



E = -438.427398 E0 = -438.228331

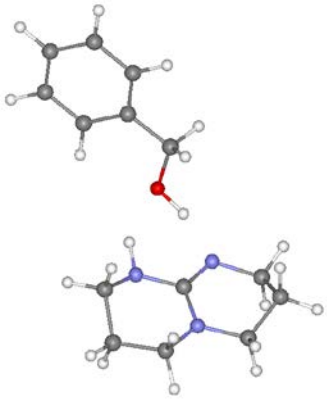
ZPVE = 0.199066 a.u. = 124.9161 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	17.9812	40.7006	0.8887	1.4812	-10.6536
rotational	13.2075	29.2270	0.8887	0.8887	-7.8253
vibrational	4.6650	22.0779	128.7347	128.7347	122.1522
total	35.8537	92.0055	130.5122	131.1047	103.6732

cartesian

7	3.19864464	0.38259727	-1.06576359	1	2.69115257	-2.49998903	0.13395593
6	1.86227262	0.07862483	-0.83816952	1	3.43293142	-1.87536371	-2.78080964
7	1.47631967	-1.24001634	-1.11084974	1	4.45683670	-2.74363208	-1.60789239
6	2.43183088	-2.32583356	-0.93142748	1	4.72381926	-0.80607915	-0.20741586
6	3.68863583	-1.96446836	-1.71476758	1	5.01710272	-0.25858685	-1.86994445
6	4.23720074	-0.64200687	-1.19157422	1	4.67983770	1.60961974	-0.24444368
6	2.73282576	2.45273709	0.21314368	1	3.84655428	2.30877233	-1.64577591
6	1.30501068	2.30021453	-0.31599018	1	2.78994393	2.01204753	1.22095180
7	0.92816734	0.90749139	-0.49022990	1	3.02699542	3.51012921	0.29122615
6	3.69228816	1.72250402	-0.72196871	1	1.20816970	2.84765959	-1.27497804
1	0.54268676	-1.39329422	-0.73545367	1	0.58907825	2.76927805	0.37648466
1	1.98127770	-3.25064492	-1.31837726				

TBD-BnOH_complex



E = -784.916253 E0 = -784.586735

ZPVE = 0.329519 a.u. = 206.7763 kcal mol^{-1}

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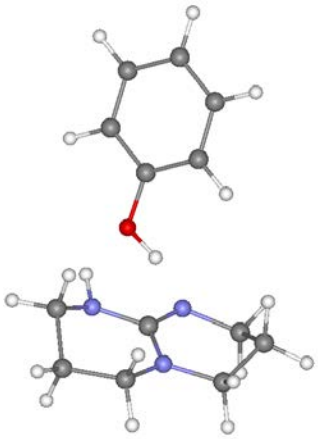
translational	18.8434	42.4139	0.8887	1.4812	-11.1645
rotational	15.5600	33.9018	0.8887	0.8887	-9.2191
vibrational	17.9454	66.8770	216.0832	216.0832	196.1438
total	52.3488	143.1927	217.8606	218.4531	175.7602

cartesian

7	1.82781470	-0.04222567	-0.04195745	1	1.06726646	-2.63659382	-1.62661183
6	0.51350325	-0.06743744	-0.46259612	1	-0.20801601	-3.22456288	-0.55424714
7	-0.11233183	1.14959073	-0.65513957	8	-2.64456797	-0.26335371	-1.16856062
6	0.36159191	2.35362744	0.00644118	6	-3.43240643	-0.55682147	-0.02677897
6	1.87023056	2.43764520	-0.19835123	1	-2.80208182	-0.62066197	0.88310319
6	2.51787186	1.18118811	0.37251979	1	-3.92341328	-1.54568267	-0.13369878
6	1.53938901	-2.44564438	0.47830966	6	-4.50745964	0.48718992	0.19669545
6	0.53747076	-2.42509365	-0.67661291	1	-1.77109897	-0.78763920	-1.08477640
7	-0.16249137	-1.15299535	-0.75259143	1	-1.11976862	1.04126966	-0.82215518
6	2.51834202	-1.28892577	0.30640426	6	-5.31221581	0.42328277	1.34472072
1	-0.14560850	3.21631336	-0.44621304	6	-4.72961617	1.51431036	-0.72780168
1	0.12778480	2.36216354	1.09042287	6	-5.73672819	2.46052980	-0.50679767
1	2.08278871	2.52085948	-1.27425766	1	-4.10743046	1.55643070	-1.62111068
1	2.28866291	3.32097268	0.30424905	6	-6.31604004	1.36674595	1.56636071
1	2.53249502	1.23779285	1.47936511	1	-5.14854145	-0.37456247	2.07373548
1	3.56826949	1.10917091	0.04450234	1	-5.90090370	3.25431228	-1.23753023
1	3.07772589	-1.11759162	1.24174678	6	-6.53257322	2.39197755	0.63851815
1	3.26285100	-1.52769029	-0.47460330	1	-6.93161631	1.30378544	2.46505117
1	0.99362278	-2.33536410	1.42813206	1	-7.31693602	3.13032699	0.80953324
1	2.09463787	-3.39424515	0.51580548				

TBD-PhOH_complex



E = -745.658504 E0 = -745.356936

ZPVE = 0.301569 a.u. = 189.2371 kcal mol^{-1}

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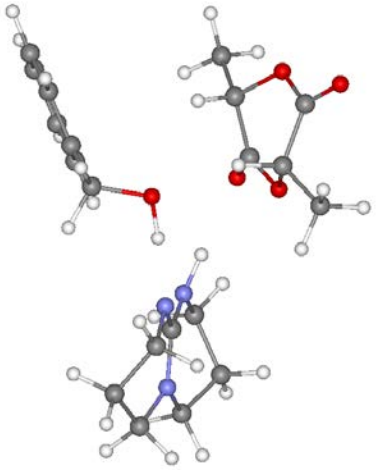
translational	18.7558	42.2399	0.8887	1.4812	-11.1126
rotational	15.2683	33.3222	0.8887	0.8887	-9.0463
vibrational	15.3013	58.5001	197.6131	197.6131	180.1713
total	49.3254	134.0622	199.3906	199.9830	160.0124

cartesian

7	1.93879175	-0.06677530	-0.12525609	1	1.18065429	-2.37937975	1.34446990
6	0.59227031	-0.02537534	-0.41120794	1	2.12540245	-3.44639301	0.27939498
7	0.00129731	1.22050047	-0.50012749	1	0.89366460	-2.58677602	-1.70648909
6	0.59075618	2.38158441	0.14780994	1	-0.27875245	-3.14606547	-0.50924236
6	2.07205677	2.41372132	-0.21176004	8	-2.62823629	-0.22159716	-0.80087036
6	2.72315097	1.11350393	0.24618620	6	-3.44946814	-0.53897893	0.23226009
6	1.60997653	-2.47673678	0.33541945	1	-1.71279263	-0.72258341	-0.74615991
6	0.48722845	-2.37885070	-0.69762224	1	-1.01747477	1.16514075	-0.56372070
7	-0.15400963	-1.07400644	-0.66445625	6	-4.68671608	0.12451438	0.32980716
6	2.61128688	-1.35320091	0.08920775	6	-3.11802197	-1.50260568	1.20520616
1	0.07661508	3.27834105	-0.22312774	6	-4.00645590	-1.78579736	2.24504614
1	0.46833941	2.35824227	1.24902940	1	-2.16132736	-2.02246261	1.13813734
1	2.17489529	2.52894807	-1.30062115	6	-5.56546688	-0.16864799	1.37191892
1	2.57666564	3.26138639	0.27244580	1	-4.94039011	0.86470944	-0.43003705
1	2.86167574	1.12951481	1.34516978	1	-3.73377562	-2.53677440	2.98891306
1	3.72635508	1.01091504	-0.19954976	6	-5.23431110	-1.12438929	2.33926988
1	3.28459549	-1.24275327	0.95553827	1	-6.52160835	0.35467547	1.42778242
1	3.24539638	-1.58690596	-0.78500974	1	-5.92462301	-1.35217154	3.15143776

I-1_LA_TBD_BnOH



E = -1318.900478 E0 = -1318.435184

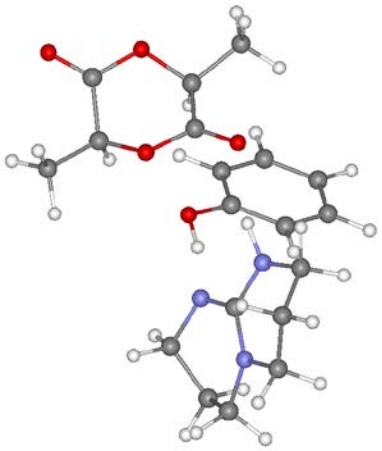
ZPVE = 0.465294 a.u. = 291.9767 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.6603	36.0885	0.8887	0.8887	-9.8711
vibrational	35.5991	127.2562	308.8261	308.8261	270.8847
total	71.7916	207.1273	310.6036	311.1960	249.4410

cartesian

7	-3.69334340	-0.67761034	-0.40898696	6	0.68640614	2.50593233	0.30371618
6	-2.33277178	-0.47269630	-0.30035263	1	-0.15123543	0.98492479	-0.69044256
7	-1.62764955	-1.31368089	0.52704954	1	-0.37810528	2.76454258	0.45548278
6	-2.23559284	-2.43365836	1.23156428	1	1.17734778	3.38332605	-0.15233114
6	-3.41530704	-2.97938442	0.43367881	8	4.21583462	-1.04971111	-1.26063609
6	-4.38028622	-1.83250403	0.16622132	6	3.75735688	-0.85083938	-2.52887583
6	-3.82049704	1.64649904	-1.25294101	6	1.69724703	-0.74298096	-4.00879955
6	-2.46674967	1.28083575	-1.86444259	1	2.08785605	0.48789027	-2.26432252
7	-1.68338430	0.47370395	-0.94008607	1	3.07616091	0.31152949	-0.15062603
6	-4.57865334	0.35846648	-0.95089716	6	3.94302011	-1.21181595	1.12411380
1	-0.62615526	-1.38972032	0.33633578	8	4.50851631	-0.92209530	-3.47575974
1	-1.45917368	-3.19571638	1.37718582	1	4.89346027	-0.67940438	1.25004148
1	-2.58288288	-2.12535048	2.23542786	1	4.13349152	-2.29218984	1.11732411
1	-3.05602312	-3.40238595	-0.51644754	1	3.28756380	-0.97553253	1.97009087
1	-3.93298411	-3.77346945	0.99015170	1	2.21895099	-0.08312142	-4.71177912
1	-4.88949299	-1.54130554	1.10625362	1	0.62837768	-0.49732903	-4.01036739
1	-5.16900158	-2.14312100	-0.54011738	1	1.83557081	-1.77841365	-4.34354305
1	-5.38716125	0.54471111	-0.22118014	6	1.32825565	2.22904515	1.65147686
1	-5.05790806	-0.02913883	-1.86809564	6	2.45449853	2.94649720	2.07516551
1	-3.64770079	2.21361661	-0.32579064	6	0.81021404	1.23136783	2.49297333
1	-4.42050457	2.27505064	-1.92700100	6	3.05330348	2.68007660	3.31154513
1	-2.63191271	0.74525082	-2.82136941	1	2.86854076	3.72232342	1.42682266
1	-1.88967741	2.18480420	-2.10743642	6	1.40414858	0.96244311	3.72689533
8	1.26370645	-1.98936129	0.43349528	1	-0.05962157	0.65600717	2.16817617
6	1.94171762	-1.45061398	-0.42470241	1	3.93134093	3.24702120	3.62457323
8	1.52346826	-1.42699385	-1.70808554	6	2.52883673	1.68640506	4.14078331
6	3.28236341	-0.77269483	-0.16552275	1	2.99373984	1.47378325	5.10428810
6	2.26419163	-0.54389381	-2.61997318	1	0.99151039	0.18302199	4.36942005
8	0.78677022	1.39765990	-0.58934361				

I-1_LA_TBD_PhOH



E = -1279.642880 E0 = -1279.205861

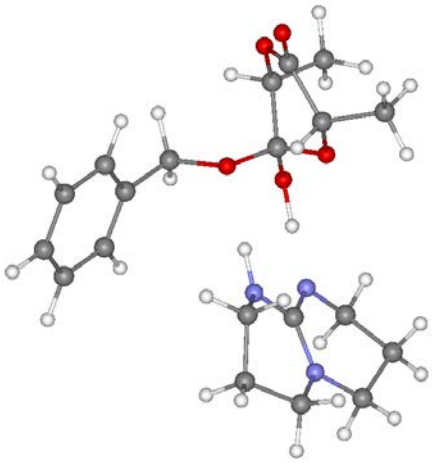
ZPVE = 0.437019 a.u. = 274.2336 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.4774	43.6739	0.8887	1.4812	-11.5402
rotational	16.5520	35.8732	0.8887	0.8887	-9.8069
vibrational	32.0139	116.8136	290.0937	290.0937	255.2657
total	68.0433	196.3607	291.8711	292.4636	233.9187

cartesian

7	-3.43062377	-0.69918782	-0.87083602	6	2.92427993	-0.43777317	-1.93032765
6	-2.10460973	-0.55108541	-0.52501827	8	0.90802288	1.39603138	-0.11070898
7	-1.54865825	-1.50649786	0.28249577	6	0.91310191	1.96007836	1.12030828
6	-2.27665019	-2.66269565	0.78016829	1	-0.02780273	0.93851089	-0.35425955
6	-3.33113050	-3.08511138	-0.23754230	8	4.54175138	-0.96304607	-0.19074605
6	-4.21909380	-1.88431120	-0.53511721	6	4.36845112	-0.72638559	-1.52232432
6	-3.40571022	1.71464241	-1.41814554	6	2.68257999	-0.59546822	-3.41570520
6	-1.96728301	1.41151071	-1.83825612	1	2.65550137	0.57942855	-1.59285533
7	-1.35292923	0.45131519	-0.93079460	1	3.17260122	0.34557846	0.69640231
6	-4.20055580	0.41427031	-1.43613768	6	3.75481606	-1.22069168	2.06853628
1	-0.52717215	-1.54430628	0.32113793	8	5.30929279	-0.75570500	-2.28290558
1	-1.54836607	-3.46370029	0.96140575	1	4.64189100	-0.68202710	2.42258668
1	-2.76429558	-2.44015884	1.74789560	1	3.96362424	-2.29758000	2.06461501
1	-2.83793187	-3.42982554	-1.15872967	1	2.92259860	-1.02760553	2.75480270
1	-3.94598198	-3.90852737	0.15208229	1	3.33359504	0.09506106	-3.96439624
1	-4.86824799	-1.66976702	0.33641824	1	1.63603461	-0.36420658	-3.64789987
1	-4.88787365	-2.09737778	-1.38608980	1	2.91328621	-1.61677909	-3.74244261
1	-5.13321829	0.52068484	-0.85438156	6	1.98694277	2.80348182	1.47010589
1	-4.49420691	0.15698001	-2.46993494	6	-0.09635571	1.72124326	2.07621408
1	-3.39680171	2.14198542	-0.40427032	6	-0.02415752	2.31603503	3.33721137
1	-3.88213515	2.44427514	-2.08865762	1	-0.92617989	1.06119215	1.82151592
1	-1.96113229	1.03407145	-2.88023162	6	2.04964542	3.38622665	2.73660159
1	-1.35643911	2.32546902	-1.83018672	1	2.75676036	3.00636268	0.72333264
8	1.30795181	-1.98944521	0.78613305	1	2.88955975	4.03750610	2.98448467
6	2.14752817	-1.41790986	0.11138779	6	1.04564285	3.14889169	3.68098736
8	2.02169776	-1.36189342	-1.23156822	1	1.09555125	3.60666990	4.66881037
6	3.38746738	-0.73747867	0.68100333	1	-0.81463349	2.11904621	4.06382227

I-2_LA_TBD_BnOH



E = -1318.891044 E0 = -1318.424915

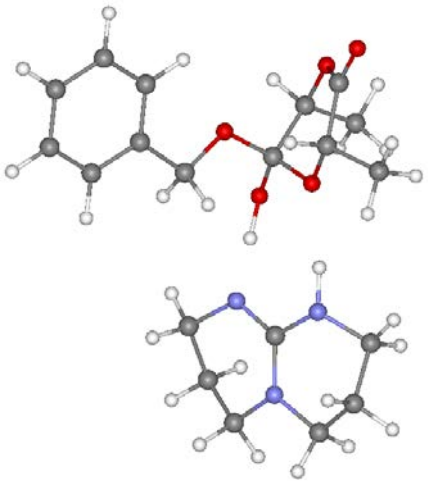
ZPVE = 0.466129 a.u. = 292.5002 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.5550	35.8791	0.8887	0.8887	-9.8086
vibrational	30.1591	112.8476	308.2768	308.2768	274.6312
total	66.2462	192.5093	310.0542	310.6467	253.2501

cartesian

7	-3.36069846	0.57198596	0.68374062	6	1.81585360	-0.26838198	-1.97223437
6	-2.06446338	0.67748255	0.22869328	1	-0.38317361	-0.36851665	-0.22508964
7	-1.46135771	1.82097113	-0.01071095	1	1.36391377	0.58152586	-2.50780773
6	-2.20116925	3.05539274	0.19992489	1	2.90715957	-0.25580385	-2.13191342
6	-3.15353632	2.93380070	1.38815296	8	4.15561342	0.49274066	0.41829169
6	-4.09135342	1.75673747	1.14659393	6	3.72422695	-0.28420898	1.44652700
6	-3.33939147	-1.87155330	0.24889387	6	2.38775706	0.20171213	3.52345872
6	-1.83343697	-1.77234757	0.45940882	1	1.81474853	-1.04945397	1.85881114
7	-1.38794446	-0.48462865	-0.04504517	1	3.55492091	1.58625984	-1.18340540
6	-4.01460218	-0.70790350	0.96480715	6	3.64193678	2.88329959	0.53138524
1	-0.02890461	1.94166601	-0.26644930	8	4.45188284	-1.15440941	1.88195419
1	-1.47331095	3.86296654	0.36533096	1	4.71938896	3.07132483	0.43715259
1	-2.77555013	3.32909465	-0.70681643	1	3.36837268	2.88725853	1.59419477
1	-2.56659126	2.76457787	2.30360913	1	3.09072113	3.68655062	0.02810857
1	-3.74362969	3.85103941	1.52731097	1	2.93385243	-0.60402811	4.02744007
1	-4.86522770	2.02605414	0.40482098	1	1.36991656	0.26105720	3.92993593
1	-4.61781216	1.48652220	2.07748318	1	2.89636445	1.15577185	3.71577191
1	-5.06961918	-0.62607610	0.65422869	6	1.24674642	-1.57687342	-2.46069407
1	-4.01621342	-0.88805866	2.05772495	6	0.03019822	-1.61735022	-3.15559006
1	-3.55695915	-1.83457601	-0.82865286	6	1.92382324	-2.77915859	-2.20565438
1	-3.73123813	-2.81855464	0.64510870	6	1.39436579	-3.99735641	-2.63613462
1	-1.59357727	-1.90511286	1.53329206	1	2.87151718	-2.75538588	-1.66437590
1	-1.30193818	-2.55669022	-0.09594771	6	-0.49930194	-2.83502865	-3.59254026
8	1.03462231	2.14292073	-0.46844789	1	-0.50480562	-0.68659317	-3.35265636
6	1.81211436	1.17302060	0.03725544	1	1.93178642	-4.92463827	-2.43381476
8	1.53467870	0.96517891	1.42039669	6	0.18141255	-4.02768755	-3.33224750
6	3.29766822	1.55011690	-0.11598185	1	-1.44332469	-2.85202074	-4.13891459
6	2.31837177	-0.08123222	2.02434421	1	-0.22888167	-4.97840166	-3.67501736
8	1.53406489	-0.15499786	-0.55800712				

I-3_LA_TBD_BnOH



E = -1318.889634 E0 = -1318.423357

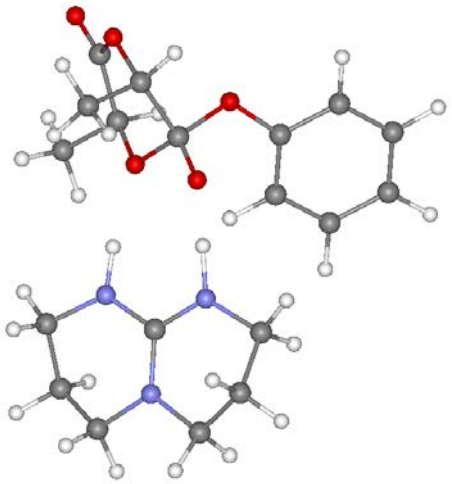
ZPVE = 0.466276 a.u. = 292.5928 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.7122	36.1916	0.8887	0.8887	-9.9018
vibrational	30.2461	113.1846	308.4183	308.4183	274.6724
total	66.4905	193.1588	310.1958	310.7883	253.1980

cartesian

7	-3.79768109	0.70009750	-0.40081918	1	-0.65477610	1.50486958	-0.42673379
6	-2.43184614	0.54412591	-0.46901044	8	3.84488201	0.66243333	-1.63540423
7	-1.82399070	-0.60252059	-0.67629683	6	3.70295191	1.47875321	-0.56437719
6	-2.64277744	-1.79907966	-0.81133884	8	4.67493010	2.05546618	-0.11717936
6	-3.95717406	-1.49631155	-1.52933311	1	2.44345379	1.12334180	1.08416045
6	-4.69497538	-0.40192133	-0.76677883	1	3.10752749	-1.01446545	-2.51438046
6	-3.51882935	3.05019546	0.36343184	6	1.25371826	-1.56908202	0.80042088
6	-2.19248033	2.99711585	-0.38684025	1	0.51802576	-2.24998379	0.34060517
7	-1.65273678	1.65489519	-0.24579480	1	0.68879008	-0.71968699	1.22686303
6	-4.45622683	1.99567175	-0.21389404	6	2.24059081	0.73034662	-3.46273422
1	-0.42448100	-0.65704381	-1.24460804	1	1.48493838	0.14563021	-3.99982238
1	-2.06063557	-2.54828882	-1.36707377	1	3.09771490	0.90773392	-4.12486124
1	-2.85792685	-2.23958254	0.18188176	1	1.80177152	1.69746530	-3.18287086
1	-3.73763227	-1.15783668	-2.55335665	6	1.99150646	3.09594154	0.33347252
1	-4.59450436	-2.38956308	-1.59746265	1	2.81226730	3.58264518	0.87180471
1	-5.16065502	-0.81454253	0.14634219	1	1.07421410	3.17768979	0.93204105
1	-5.50890064	0.01538667	-1.38301420	1	1.84136951	3.61077905	-0.62526721
1	-5.32192421	1.84663320	0.45263961	6	2.00300694	-2.28556299	1.90109861
1	-4.85768890	2.34190512	-1.18616831	6	1.27191484	-3.01301217	2.85289741
1	-3.33620429	2.85647821	1.43048453	6	3.39726114	-2.23072958	2.01512218
1	-3.98676085	4.04002857	0.27009764	6	4.04595852	-2.88905358	3.06541872
1	-2.34513736	3.27919912	-1.44748759	1	3.97163105	-1.67593169	1.27450311
1	-1.46960282	3.70506859	0.04054061	6	1.91890419	-3.66567421	3.90269184
8	0.48624542	-0.77290714	-1.80432367	1	0.18388632	-3.06903172	2.76842189
6	1.58385050	-0.26796442	-1.19978571	1	5.13313198	-2.83924937	3.14037514
8	1.23976576	1.02738881	-0.61593354	6	3.31228757	-3.60566807	4.01278877
6	2.70149088	-0.03346866	-2.23280740	1	3.82080746	-4.11774158	4.83043957
6	2.33117938	1.62641323	0.10713813	1	1.33567142	-4.22736979	4.63379097
8	2.16990852	-1.10042644	-0.19371378				

I-3_LA_TBD_PhOH



E = -1279.622580 E0 = -1279.184505

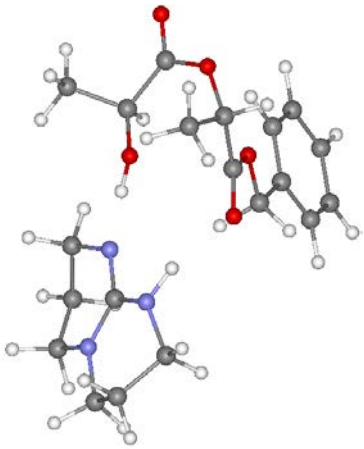
ZPVE = 0.438075 a.u. = 274.8962 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.4774	43.6739	0.8887	1.4812	-11.5402
rotational	16.4363	35.6433	0.8887	0.8887	-9.7383
vibrational	27.4439	104.9360	289.9227	289.9227	258.6360
total	63.3577	184.2532	291.7001	292.2926	237.3576

cartesian

7	-3.30307317	0.61110473	-0.62170547	6	2.65848160	1.45523751	0.62195683
6	-1.95641994	0.39479816	-0.62991405	8	2.74291205	-1.28911841	0.40985402
7	-1.44084048	-0.82917869	-0.59534049	1	-0.10175501	1.24712765	-0.54718447
6	-2.28974724	-2.00626421	-0.50332487	8	4.24412632	0.58975971	-1.10199714
6	-3.58908272	-1.76415801	-1.26746655	6	4.03416348	1.42119968	-0.05771172
6	-4.25623751	-0.50024641	-0.73493856	8	4.95039797	2.10472202	0.35998335
6	-2.88127160	2.97837543	-0.02321011	1	2.81132913	0.94483626	1.59051836
6	-1.56966209	2.82220840	-0.78719962	1	3.66562676	-1.18481612	-1.90785646
7	-1.10892522	1.44909704	-0.66526979	6	2.01837730	-1.94343829	1.36748528
6	-3.88562751	1.95414340	-0.53995633	6	2.67566824	0.43443549	-2.94953561
1	-0.34304491	-0.94820952	-0.78523469	1	1.96892655	-0.23061433	-3.45944095
1	-1.72945869	-2.85151100	-0.92243397	1	3.52486706	0.64050472	-3.61379790
1	-2.50506496	-2.25061750	0.55227721	1	2.16734076	1.38209546	-2.72298861
1	-3.36506438	-1.64909971	-2.33843064	6	2.21600652	2.89308190	0.87652552
1	-4.27738810	-2.61280060	-1.15410447	1	2.99785590	3.42675447	1.42822921
1	-4.70955610	-0.69112611	0.25420532	1	1.29171658	2.89882183	1.47079062
1	-5.06718874	-0.17875391	-1.40819418	1	2.03863406	3.41765499	-0.07329229
1	-4.75905800	1.90220273	0.12972343	6	2.55799127	-3.15246940	1.84052467
1	-4.25857449	2.25242400	-1.53689301	6	0.83029163	-1.45700991	1.94120812
1	-2.69869399	2.82056832	1.05001009	6	0.20263541	-2.17892337	2.96107316
1	-3.29220104	3.98852038	-0.15435573	1	0.41520041	-0.51221597	1.59776962
1	-1.71127868	3.10243177	-1.84703898	6	1.92894244	-3.85734248	2.86550498
1	-0.79088950	3.47827435	-0.37725985	1	3.48035622	-3.51767564	1.38865602
8	1.01019704	-1.13554299	-1.20198071	1	2.36755300	-4.79089308	3.22151375
6	2.02665424	-0.53512025	-0.68369722	6	0.74146307	-3.37911844	3.43093228
8	1.61948895	0.78538179	-0.10498434	1	-0.71547961	-1.78578603	3.40256715
6	3.16989064	-0.23259369	-1.67601073	1	0.24849401	-3.93112063	4.23143911

I-4_LA_TBD_BnOH



E = -1318.888720 E0 = -1318.422910

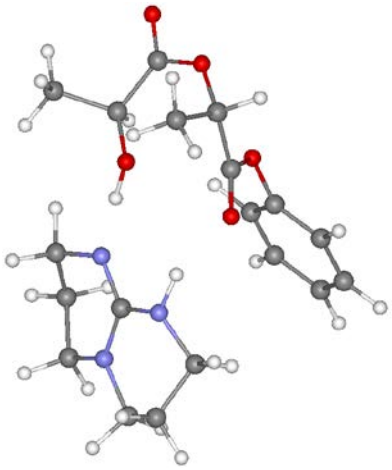
ZPVE = 0.465810 a.u. = 292.3000 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.6548	36.0774	0.8887	0.8887	-9.8678
vibrational	32.2034	119.3020	308.7897	308.7897	273.2198
total	68.3903	199.1621	310.5672	311.1597	251.7795

cartesian

7	3.52222610	0.13432124	0.88821417	1	-0.28606120	0.36266631	1.45156860
6	2.17906737	-0.17633566	0.92383349	8	-3.91036606	-0.69864517	1.23990679
7	1.84294748	-1.49464512	1.13627005	6	-3.57821560	0.62842679	1.35567367
6	2.79733157	-2.56972504	0.91722041	8	-4.49582720	1.42199862	1.29015017
6	4.11331606	-2.17723155	1.57670689	1	-1.90460789	1.55418432	0.50563222
6	4.59149551	-0.86343646	0.97118974	1	-3.69452620	-2.61812782	0.76426291
6	2.85272884	2.30103254	-0.09204376	6	-1.04671144	-0.85848236	-1.75829244
6	1.57753038	2.10837197	0.72602260	1	-0.73489201	-1.86720288	-2.06411362
7	1.20534420	0.70189929	0.81958038	1	-0.18366209	-0.37132210	-1.27227628
6	3.97133374	1.48756886	0.54653400	6	-2.68074560	-2.34187078	2.62908840
1	0.86080599	-1.71656573	0.95394892	1	-2.16422343	-3.30764747	2.55978823
1	2.38534856	-3.48426127	1.36368346	1	-3.60300303	-2.47743654	3.20813847
1	2.96108389	-2.77191830	-0.16041714	1	-2.02495909	-1.62219059	3.12894082
1	3.95492959	-2.06383610	2.65914392	6	-2.09389377	2.27963781	2.53060436
1	4.87906837	-2.94971538	1.42047000	1	-2.82576776	3.05561805	2.27844095
1	5.00515175	-1.04318380	-0.04062128	1	-1.08718884	2.71841884	2.54518032
1	5.40815926	-0.43646386	1.57694852	1	-2.31486177	1.89153624	3.53399420
1	4.82529593	1.39588070	-0.14574277	6	-1.53052187	-0.05193153	-2.93820214
1	4.34608316	1.99294543	1.45526469	6	-0.83613443	-0.16255066	-4.15229893
1	2.67603040	1.95323086	-1.12143683	6	-2.61640739	0.82943881	-2.85446310
1	3.14582944	3.35965633	-0.13811404	6	-1.20913649	0.60225284	-5.25869465
1	1.72052610	2.54356885	1.73538089	1	0.00322726	-0.85713577	-4.23247147
1	0.74256867	2.65787911	0.26642507	6	-2.99423647	1.58866739	-3.96615338
8	-0.85595965	-2.48387289	0.37051716	1	-3.17532921	0.91497421	-1.92344093
6	-1.84600413	-1.77034009	0.28031716	1	-3.84499836	2.26657414	-3.88779950
8	-1.21004570	0.11311483	1.83152890	6	-2.29175568	1.48246062	-5.16854954
6	-3.03867102	-1.85953486	1.23059273	1	-2.58970094	2.07607579	-6.03338718
6	-2.13095546	1.13454628	1.50737858	1	-0.66019678	0.50289935	-6.19599438
8	-2.10785866	-0.96423674	-0.77402925				

I-4_LA_TBD_PhOH



E = -1279.615937 E0 = -1279.178331

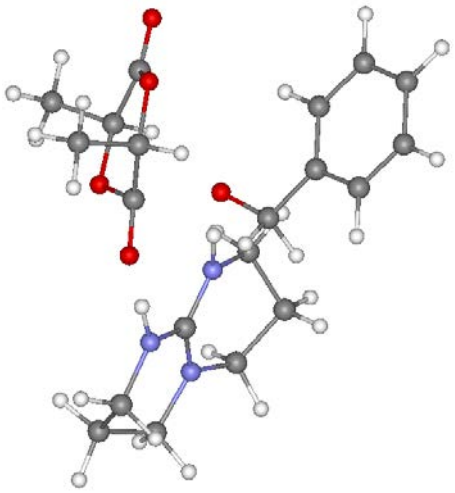
ZPVE = 0.437606 a.u. = 274.6020 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.4774	43.6739	0.8887	1.4812	-11.5402
rotational	16.3559	35.4835	0.8887	0.8887	-9.6907
vibrational	30.5789	113.1186	290.2106	290.2106	256.4843
total	66.4122	192.2760	291.9881	292.5806	235.2535

cartesian

7	3.05205560	0.59691346	0.51672512	6	-2.62563586	1.50023222	1.01866210
6	1.71842682	0.27444988	0.66944200	8	-2.32804251	-0.91760063	-1.17085862
7	1.40345693	-1.06289184	0.74119663	1	-0.76893771	0.74743658	1.17414606
6	2.30575347	-2.08802748	0.23971528	8	-4.37907124	-0.30556357	0.48797089
6	3.70049667	-1.78819239	0.77398890	6	-4.02737856	1.01772678	0.60028213
6	4.10985899	-0.39549017	0.31148550	8	-4.88504076	1.83046961	0.32102755
6	2.28935504	2.87891030	-0.05996731	1	-2.26098704	2.01742053	0.10788704
6	1.13390231	2.55847597	0.88651377	1	-4.19473028	-2.27622914	0.32329896
7	0.75307441	1.15520322	0.80771112	6	-1.26034522	-1.03490031	-2.07453322
6	3.47105312	1.98367763	0.29112262	6	-3.47210360	-1.77431870	2.27417421
1	0.40733358	-1.28049874	0.69128871	1	-3.01401448	-2.76105213	2.41774368
1	1.94127893	-3.06015873	0.59607983	1	-4.47888279	-1.78707182	2.71069217
1	2.32305026	-2.12445617	-0.86726719	1	-2.85193062	-1.02311587	2.77310109
1	3.68663621	-1.83776498	1.87265611	6	-2.77238107	2.54466724	2.13906050
1	4.43125725	-2.52193236	0.40597686	1	-3.47041869	3.33790398	1.84630632
1	4.38274670	-0.42214677	-0.76187485	1	-1.78956580	2.98450637	2.35518789
1	5.00509930	-0.05574917	0.85888928	1	-3.13948345	2.06128192	3.05467153
1	4.21197939	1.98617733	-0.52659011	6	-0.68754888	0.14842519	-2.53954005
1	3.98660016	2.36230087	1.19249046	6	-0.85082877	-2.27646708	-2.56514335
1	1.96829224	2.68913388	-1.09567189	6	0.31365278	0.08844905	-3.51180315
1	2.59187913	3.93358469	0.01289329	1	-1.03265274	1.10053921	-2.13902664
1	1.42154121	2.83033705	1.92197514	6	0.15499964	-2.32455397	-3.53330636
1	0.25550303	3.17288089	0.63853180	1	-1.31320417	-3.18891168	-2.19372916
8	-1.33191681	-2.28815031	0.37873828	1	0.47848710	-3.29128504	-3.92050600
6	-2.25381613	-1.57127988	0.03732133	6	0.73980188	-1.14657187	-4.00831270
8	-1.74477184	0.46144357	1.38582158	1	1.51975274	-1.19157565	-4.76874065
6	-3.58181262	-1.47901189	0.78495836	1	0.75818062	1.01242030	-3.88286543

TS-12_LA_TBD_BnOH



E = -1318.885431 E0 = -1318.421483

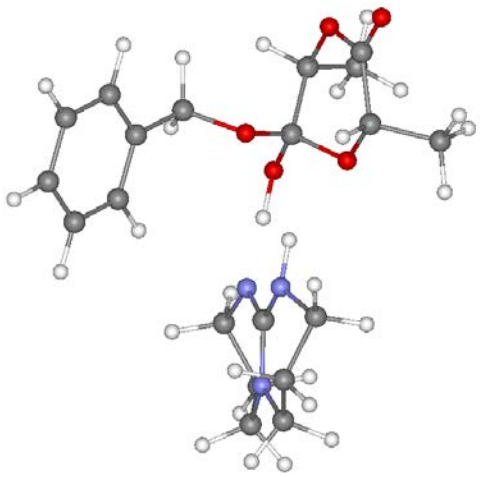
ZPVE = 0.463948 a.u. = 291.1317 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.6056	35.9797	0.8887	0.8887	-9.8386
vibrational	29.7842	111.9566	306.8648	306.8648	273.4850
total	65.9219	191.7189	308.6423	309.2348	252.0738

cartesian

7	-3.75324869	-0.32416147	-0.75144958	6	0.70385540	0.67266715	1.66239822
6	-2.43041706	-0.48546275	-0.43630397	1	-0.46723676	0.41505790	-0.22636463
7	-2.00674677	-1.66095376	0.06916350	1	0.76930845	-0.28857106	2.21580076
6	-2.91404986	-2.75669193	0.36514080	1	-0.31175157	1.06472206	1.89422667
6	-4.03024769	-2.78369975	-0.67374051	8	3.60727501	-0.37504405	-0.54679954
6	-4.71924591	-1.42455292	-0.68763953	6	3.11680484	0.12020385	-1.70214128
6	-3.36540866	2.12213731	-0.73742265	6	1.94887209	-0.93621778	-3.65999031
6	-1.96245933	1.75916386	-1.21568477	1	1.13627338	0.51334763	-2.27400541
7	-1.54757106	0.49569505	-0.62683570	1	2.91184211	-0.93393874	1.28366745
6	-4.31421852	0.98600316	-1.10045934	6	3.51913309	-2.68783379	0.17014444
1	-0.97696018	-1.81643713	0.22187793	8	3.74456072	0.96468008	-2.31231022
1	-2.32867670	-3.68506241	0.34930336	1	4.57979631	-2.59007263	0.43450814
1	-3.34398675	-2.65698695	1.37923110	1	3.44432235	-3.09831572	-0.84612834
1	-3.60224867	-3.00213766	-1.66322029	1	3.03614378	-3.38209343	0.86854410
1	-4.76773596	-3.56383014	-0.44044045	1	2.40503454	-0.17569822	-4.30380821
1	-5.35030794	-1.30695081	0.21293777	1	0.96691859	-1.21426392	-4.06384039
1	-5.38581944	-1.33845186	-1.56147778	1	2.58900547	-1.82865322	-3.65145636
1	-5.27182865	1.09618044	-0.56491375	6	1.71961164	1.64773059	2.24250412
1	-4.54371405	1.00713086	-2.18126011	6	1.82745266	1.78812122	3.63514709
1	-3.34898973	2.26915860	0.35277808	6	2.53853512	2.43064260	1.42138922
1	-3.71730876	3.05377674	-1.20146108	6	2.72893667	2.69434571	4.19547033
1	-1.94584882	1.70644045	-2.32065105	1	1.19926167	1.17527258	4.28732538
1	-1.22789657	2.51990843	-0.91899025	6	3.44669294	3.33606315	1.98099983
8	0.62885261	-2.14590406	0.59311521	1	2.46593213	2.31404614	0.34061635
6	1.36729801	-1.42602563	-0.10738853	1	2.80212140	2.78837276	5.28026724
8	1.10115254	-1.38848782	-1.46608281	6	3.54447603	3.47401452	3.36733150
6	2.84281731	-1.32057571	0.25859582	1	4.25487041	4.17836571	3.80214834
6	1.78035498	-0.38002953	-2.24821138	1	4.08450937	3.93205047	1.32638192
8	0.82191622	0.45180374	0.27946168				

TS-23_LA_TBD_BnOH



E = -1318.889134 E0 = -1318.422719

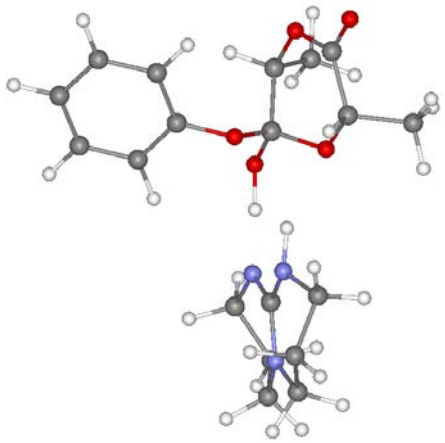
ZPVE = 0.466415 a.u. = 292.6798 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.5958	35.9603	0.8887	0.8887	-9.8328
vibrational	29.2339	109.6836	308.0612	308.0612	275.3591
total	65.3619	189.4265	309.8387	310.4312	253.9537

cartesian

7	-3.39367652	-0.48919442	-0.65743041	6	1.93201196	0.60059899	1.97962630
6	-2.05031228	-0.52069873	-0.35355699	1	-0.23522015	0.16527790	-0.88092881
7	-1.51500797	-1.28644097	0.56911707	8	4.29245234	-0.80692548	-0.25913194
6	-2.39828324	-2.14466429	1.34577882	6	3.97119617	-0.19228575	-1.42576420
6	-3.55193877	-2.67334890	0.49502826	6	2.50313401	-0.74229407	-3.39857960
6	-4.30893517	-1.49075651	-0.09821001	1	2.19034290	0.79695874	-1.91149521
6	-3.04899168	1.49144721	-2.11658287	1	3.56419539	-1.49438596	1.50515735
6	-1.62494004	0.97186679	-2.27579141	6	3.47882867	-3.08756804	0.05515289
7	-1.22784102	0.36082411	-1.01775491	8	4.82006645	0.43907171	-2.02272892
6	-3.95865488	0.33070463	-1.73207092	1	4.52537107	-3.38604712	0.19952366
1	-0.00475598	-1.57099771	0.68452245	1	3.20273972	-3.24941778	-0.99487340
1	-1.79998291	-2.97504592	1.74785757	1	2.83489466	-3.71416116	0.68330699
1	-2.80486631	-1.59836054	2.21947765	1	3.15898228	-0.11667481	-4.01455641
1	-3.14512348	-3.30156732	-0.31202093	1	1.47766376	-0.68511492	-3.78676462
1	-4.24137974	-3.29010987	1.08931494	1	2.84045911	-1.78542686	-3.46002889
1	-4.94799185	-1.01732957	0.66901124	6	1.26737189	1.92028499	2.28198791
1	-4.97605371	-1.82868552	-0.90889347	1	3.00758147	0.65835232	2.21970749
1	-4.93819237	0.70753604	-1.39399004	1	1.47355318	-0.20606732	2.57408142
1	-4.14966249	-0.30703712	-2.61739087	6	-0.13259886	2.01020074	2.33012080
1	-3.06487560	2.26479125	-1.33492696	6	2.03006196	3.07150412	2.51510453
1	-3.41070795	1.94154310	-3.05139327	6	1.41001379	4.29292059	2.79613185
1	-1.57438922	0.25961113	-3.12364364	1	3.11937499	3.00985980	2.47398329
1	-0.92860430	1.79362559	-2.49038553	6	-0.75361145	3.22884226	2.60717845
8	0.99878418	-1.89834070	0.84341127	1	-0.73018610	1.11549759	2.14319015
6	1.88173842	-1.09120893	0.21273692	1	2.01637125	5.18130732	2.97731805
8	1.61826217	-1.07604980	-1.19890273	6	0.01647897	4.37359285	2.84254265
6	3.30764103	-1.62673688	0.44455311	1	-1.84245503	3.28685784	2.64680958
6	2.53252482	-0.25219959	-1.95363259	1	-0.46975869	5.32471752	3.06341815
8	1.75689685	0.30734766	0.57627439				

TS-23_LA_TBD_PhOH



E = -1279.620996 E0 = -1279.182847

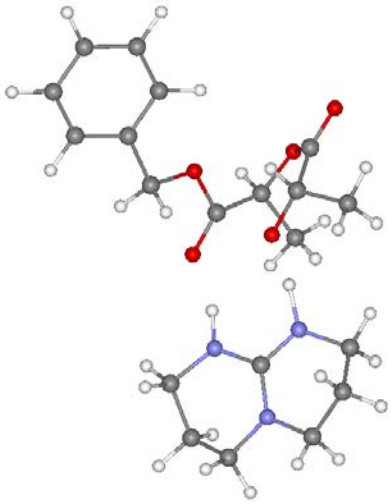
ZPVE = 0.438149 a.u. = 274.9429 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.4774	43.6739	0.8887	1.4812	-11.5402
rotational	16.4713	35.7129	0.8887	0.8887	-9.7591
vibrational	26.0600	100.3092	289.4099	289.4099	259.5026
total	62.0088	179.6961	291.1873	291.7798	238.2034

cartesian

7	-3.50376368	-0.15428787	-1.05894494	6	2.48529959	0.41779548	-1.74502087
6	-2.19050741	-0.18230054	-0.64852452	8	1.43938088	0.81725532	0.72581172
7	-1.69274521	-1.06950939	0.18230762	6	1.47866631	1.10126758	2.08514786
6	-2.58656001	-2.07474613	0.73937464	1	-0.37486368	0.64137727	-0.91245413
6	-3.64994979	-2.49513245	-0.27337119	8	4.10008144	-0.14225262	0.08290911
6	-4.41357565	-1.25704026	-0.72878253	6	3.86101127	0.51545185	-1.07733142
6	-3.14850354	2.05204058	-2.14461327	6	2.61730433	0.00806352	-3.20899129
6	-1.69416320	1.61363769	-2.26859808	1	2.08451390	1.44511473	-1.68223286
7	-1.36288702	0.82380664	-1.09322441	1	3.22548914	-0.90463066	1.74880552
6	-4.02926445	0.81397861	-2.02491593	6	3.39822674	-2.46976185	0.26697773
1	-0.23263037	-1.22119915	0.48336014	8	4.72842073	1.21772277	-1.55829251
1	-1.97870266	-2.93784904	1.04685521	1	4.44142771	-2.70659447	0.51299942
1	-3.07923269	-1.69418156	1.65539014	1	3.24220657	-2.62192869	-0.80921757
1	-3.15888858	-2.97117519	-1.13572705	1	2.73560143	-3.15016317	0.81412780
1	-4.35238647	-3.22152138	0.15975395	1	3.29369903	0.69808614	-3.72594619
1	-5.12068939	-0.92934108	0.05456689	1	1.63119745	0.03659254	-3.69079685
1	-5.01052570	-1.48209918	-1.62823665	1	3.01467705	-1.01229787	-3.28987932
1	-5.04562855	1.09705806	-1.70482194	6	2.55790377	1.84348285	2.58227110
1	-4.12954855	0.32551146	-3.01379585	6	0.42508668	0.73747301	2.93446970
1	-3.25835371	2.68679571	-1.25339353	6	2.58583641	2.21522856	3.92853355
1	-3.46016335	2.63562965	-3.02179790	1	3.36604476	2.12016058	1.90461850
1	-1.54842246	1.04727829	-3.21017766	6	0.46687424	1.10706234	4.28115273
1	-1.02219868	2.48191261	-2.29594207	1	-0.41452920	0.17478234	2.52999711
8	0.78054476	-1.46182120	0.78256977	1	-0.35373515	0.82178444	4.94112730
6	1.67138374	-0.58889973	0.29563132	6	1.54320514	1.84517539	4.78305960
8	1.54747605	-0.48854464	-1.12551880	1	3.42799354	2.79437876	4.30950880
6	3.09592175	-1.03304851	0.66511309	1	1.56694245	2.13441825	5.83410454

TS-34_LA-TBD-BnOH



E = -1318.880366 E0 = -1318.417377

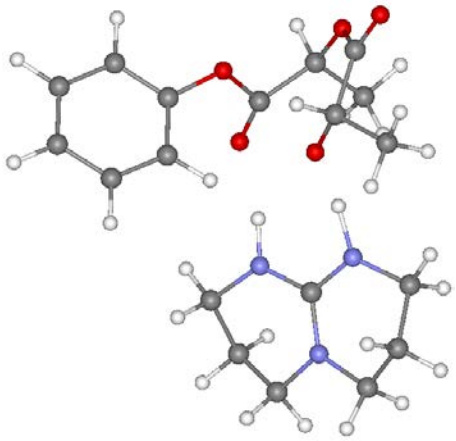
ZPVE = 0.462989 a.u. = 290.5303 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.5322	43.7826	0.8887	1.4812	-11.5726
rotational	16.7255	36.2181	0.8887	0.8887	-9.9097
vibrational	31.7637	116.4916	306.4426	306.4426	271.7107
total	68.0214	196.4923	308.2201	308.8126	250.2284

cartesian

7	-4.00815535	0.47767198	-0.51023597	1	-0.68438888	1.24424374	-0.47056544
6	-2.64580703	0.34763217	-0.55522799	8	2.95484018	0.94138384	-1.96583891
7	-2.10239339	-0.88891375	-0.56032044	6	2.83990669	1.80869496	-0.91170734
6	-2.90037274	-2.10187578	-0.48501098	8	3.75427532	2.59310389	-0.74017501
6	-4.22123098	-1.88594520	-1.21617770	1	2.08770013	1.45731449	1.00603640
6	-4.91573000	-0.66789061	-0.61991012	1	2.67398572	-0.83606303	-2.84020901
6	-3.66213679	2.82846689	0.18808565	6	1.99032855	-1.83007205	0.98022473
6	-2.41083813	2.74044466	-0.68228370	1	1.57559395	-2.79714203	0.66208160
7	-1.83949780	1.40611494	-0.59836930	1	1.18000674	-1.26137078	1.46833754
6	-4.65778208	1.77178335	-0.27473310	6	0.96051639	0.37202051	-3.28939819
1	-1.09410596	-0.99615216	-0.77908659	1	0.37245411	-0.48022962	-3.65340471
1	-2.31366134	-2.90961981	-0.94005901	1	1.44954848	0.85528934	-4.14482021
1	-3.09336782	-2.38540554	0.56601584	1	0.28843850	1.08431029	-2.79733610
1	-4.02449894	-1.72472250	-2.28644037	6	1.12602639	3.21245861	0.24549314
1	-4.87497616	-2.76327467	-1.11687052	1	1.95288420	3.86593056	0.54749000
1	-5.32211208	-0.91165662	0.37935069	1	0.35615140	3.22330856	1.03007317
1	-5.76828909	-0.36218917	-1.24847686	1	0.69390064	3.60413551	-0.68747252
1	-5.44650412	1.62408185	0.48198804	6	3.15708232	-2.02067900	1.91813290
1	-5.15843105	2.09682226	-1.20459902	6	3.16043353	-3.12575817	2.78148651
1	-3.38328195	2.65468168	1.23800480	6	4.21611214	-1.10467386	1.98423159
1	-4.12729836	3.82168770	0.12006059	6	5.25384521	-1.29228139	2.90121579
1	-2.66318202	2.99766016	-1.72842348	1	4.23258638	-0.24967819	1.30907071
1	-1.64838815	3.45682812	-0.35073447	6	4.19251966	-3.30730200	3.70456147
8	0.46259004	-1.62961066	-1.22741914	1	2.34766006	-3.85365343	2.72729945
6	1.45445633	-0.89439750	-1.12788200	1	4.18073082	-4.17324781	4.36792231
8	0.61453575	0.88908982	-0.33175981	6	5.24473190	-2.38939381	3.76669669
6	2.02028823	-0.11610076	-2.31358814	1	6.05623484	-2.53231096	4.48117208
6	1.62428975	1.76977766	0.04234752	1	6.07434797	-0.57445961	2.93742847
8	2.41742730	-1.07886589	-0.17627141				

TS-34_LA-TBD-PhOH



E = -1279.610253 E0 = -1279.175923

ZPVE = 0.434330 a.u. = 272.5462 kcal mol^{-1}

	ln(Q)	S, cal $mol^{-1}K$	U, kcal mol^{-1}	H, kcal mol^{-1}	G, kcal mol^{-1}
translational	19.4774	43.6739	0.8887	1.4812	-11.5402
rotational	16.4561	35.6826	0.8887	0.8887	-9.7500
vibrational	28.3237	106.8787	287.6306	287.6306	255.7647
total	64.2572	186.2352	289.4081	290.0006	234.4745

cartesian

7	-3.36473298	0.42323610	-0.42517537	6	2.14834690	1.80719340	0.45415601
6	-1.99853802	0.33381897	-0.46846950	8	3.03313780	-1.07733631	0.12832759
7	-1.42307663	-0.89117575	-0.46373218	1	-0.03468116	1.27324784	-0.30715495
6	-2.18695903	-2.12430382	-0.36313233	8	3.70752382	1.09697711	-1.42967749
6	-3.51291275	-1.95661294	-1.09813702	6	3.42995477	1.95550358	-0.39488098
6	-4.24077225	-0.74780285	-0.52289927	8	4.26939583	2.79670596	-0.13991845
6	-3.08183360	2.78601384	0.26273674	1	2.54699063	1.40727711	1.41489768
6	-1.83171952	2.72462201	-0.61270612	1	3.56173587	-0.60820293	-2.45873427
7	-1.21827984	1.40948403	-0.51995689	6	2.61228633	-1.92375517	1.15936804
6	-4.04997301	1.69852507	-0.18759601	6	1.88242865	0.60629410	-3.00588727
1	-0.42060465	-0.96863943	-0.69736218	1	1.35553086	-0.22339752	-3.49391580
1	-1.57922006	-2.92550492	-0.80124086	1	2.45422983	1.15829849	-3.76252842
1	-2.37172723	-2.39145041	0.69343448	1	1.14506340	1.27147722	-2.54232240
1	-3.31996989	-1.80925119	-2.17108607	6	1.58826673	3.20758414	0.75313497
1	-4.14282179	-2.84939408	-0.98330009	1	2.36305332	3.84580708	1.19322896
1	-4.64410591	-0.98781365	0.47862649	1	0.74993271	3.12119031	1.45870316
1	-5.09929609	-0.47398633	-1.15824795	1	1.23143256	3.68405437	-0.17205253
1	-4.82792521	1.53072667	0.57627970	6	3.42504144	-3.01611996	1.46390986
1	-4.56786251	2.00515938	-1.11421168	6	1.47605431	-1.63584220	1.91976786
1	-2.79344320	2.62783074	1.31260669	6	1.15392768	-2.46715665	2.99510288
1	-3.57494211	3.76547098	0.19019054	1	0.87865871	-0.76158273	1.66003180
1	-2.09675741	2.96382523	-1.66001916	6	3.09447312	-3.83730865	2.54490471
1	-1.09042597	3.46847844	-0.29256296	1	4.31034994	-3.20619559	0.85754746
8	1.19668055	-1.54514837	-1.17274559	1	0.27212995	-2.24494576	3.59795880
6	2.15911317	-0.82640851	-0.91630524	6	1.95687652	-3.56807137	3.31088829
8	1.19922996	0.93534738	-0.07708243	1	1.70140207	-4.20848751	4.15550804
6	2.83878469	0.06103846	-1.95559204	1	3.73055768	-4.68929482	2.78732347